Skills to Be Tested

1. Identify the central atom in a molecule containing more than two atoms as a start.
2. Identify the number of valence electrons of any element. This concept is important, because you need to know the number of valence electrons in order to write a Lewis dot structure for the molecule in question.
3. Count the number of VSEPR pairs or steric number (SN) for the central atom in a molecule. You need this number in order to describe or predict the shape of the molecule in question.
4. Determine the number of lone electron pairs that are not shared with other atoms. Often, a Lewis dot structure is useful to help you count this number.
5. Predict the shape of molecules or ions as the key concept of VSEPR theory. From the shape and by applying the idea that lone electron pairs take up more space, you can predict the bond angles within 5% of the observed values.
6. Predict the values of bond angles and describe the hybrid orbitals used by the central atoms in the molecules or ions.

Valence-Shell Electron-Pair Repulsion (VSEPR) Models

The 3-dimensional structure of \(\ce{BF3}\) is different from \(\ce{PF3}\), and this is difficult to comprehend by considering their formulas alone. However, the Lewis dot structures for them are different, and the electron pair in \(\ce{PF3}\) is the reason for its structure being different from \(\ce{BF3}\) (no lone pair). Three-dimensional arrangements of atoms or bonds in molecules are important properties as are bond lengths, bond angles and bond energies. The Lewis dot symbols led us to see the non-bonding electron pairs, whose role in determining the shape of a molecule was examined by N.V. Sidgwick and H.E. Powell in 1940, and later by R.S. Nyholm and R.J. Gillespie. They have developed an extensive rationale called valence-shell electron-pair repulsion (VSEPR) model of molecular geometry.

Molecular shapes and steric numbers (SN)

<table>
<thead>
<tr>
<th>Example</th>
<th>SN</th>
<th>Descriptor</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\ce{BeCl2}), (\ce{CO2})</td>
<td>2</td>
<td>Linear</td>
</tr>
<tr>
<td>(\ce{BF3}), (\ce{SO3})</td>
<td>3</td>
<td>Trigonal planar</td>
</tr>
<tr>
<td>(\ce{SO2E}), (\ce{OO2E})</td>
<td></td>
<td>bent</td>
</tr>
<tr>
<td>(\ce{CH4})</td>
<td>4</td>
<td>Tetrahedral</td>
</tr>
<tr>
<td>(\ce{NH3E})</td>
<td></td>
<td>pyramidal</td>
</tr>
<tr>
<td>(\ce{H2OE2})</td>
<td></td>
<td>bent</td>
</tr>
<tr>
<td>(\ce{PF5})</td>
<td>5</td>
<td>Trigonal bipyramidal</td>
</tr>
<tr>
<td>(\ce{SF4E})</td>
<td></td>
<td>butterfly</td>
</tr>
<tr>
<td>(\ce{ClF3E2})</td>
<td></td>
<td>T-shape</td>
</tr>
<tr>
<td>(\ce{SF6}), (\ce{OIF5})</td>
<td>6</td>
<td>Octahedral</td>
</tr>
<tr>
<td>(\ce{BrF5E})</td>
<td></td>
<td>pyramidal</td>
</tr>
<tr>
<td>(\ce{XeF4E2})</td>
<td></td>
<td>square planar</td>
</tr>
</tbody>
</table>
\(\text{\ce{E}}\) represents a lone electron pair. SN is also called the **number of VSEPR pairs** or **number of electron pairs**.

The Valence-Shell Electron-Pair Repulsion (VSEPR) models consider the unshared pairs (or lone electron pairs) and the bonding electrons. These considerations of lone and bonding electron pairs give an excellent explanation about the molecular shapes. The VSEPR model counts both bonding and nonbonding (lone) electron pairs, and calls the total number of pairs the **steric number** (SN). If the element A has \(m\) atoms bonded to it and \(n\) nonbonding pairs, then

\[
\text{SN} = m + n
\]

SN is useful for predicting shapes of molecules. If \(\text{\ce{X}}\) is any atom bonded to \(\text{\ce{A}}\) (in single, double, or triple bond), a molecule may be represented by \(\text{\ce{AX_mE_n}}\) where \(\text{\ce{E}}\) denotes a lone electron pair. This formula enables us to predict its geometry. The common SN, descriptor, and examples are given in the table on the right. Note that the SN is also called the **number of VSEPR pairs** or **number of electron pairs**. The VSEPR model has another general rule:

- **Lone pairs of electrons take up more space than bonded pairs** making the bond angle, say \(\text{\ce{\mathit{H-O-H}}}\) for water less than the tetrahedral angle of 109.5°. Actually, the \(\text{\ce{\mathit{H-O-H}}}\) angle in water is 105°.

The geometry of the molecules with their SNs equal to 2 to 6 are given in the Table 1. The first line for each is the shape including the lone electron pair(s). If the lone electron pairs are ignored, the geometry of the molecule is given by another descriptor. To get an idea about the shapes of molecules and ions, three dimensional models are the best to use. However, good computer graphics sometimes also illustrate very well. The link VSEPR Illustration: View and manipulate molecular models gives excellent graphics, and you may enjoy seeing some of the graphics of the molecules.

### Confidence Building Questions

1. **What is the central atom in \(\text{\ce{CCl2O}}\)?**

   **Hint:** Carbon is the central atom.

   **Skill:**
   Identifying the central atom is a good start to drawing a structure:
   
   \[
   \begin{array}{c}
   \text{Cl} \\
   \text{Cl} \\
   \text{C=O} \\
   \text{Cl}
   \end{array}
   \]

2. **What is the number of valence electrons in carbon?**

   **Hint:** Sulfur has 4 valence electrons.

   **Skill:**
   Give the number of valence electrons of any main-group element.
3. **What is the number of lone pair electrons around the central atom \(\text{S}\) in \(\text{SCl}_2\text{O}\)?**

Hint: There is no lone electron pair.

**Skill:**
Draw a Lewis dot structure, and express it in the form \(\text{CCl}_2\text{O}\).

This carbonyl chloride is also called phosgene, a colourless, chemically reactive, highly toxic gas having an odour like that of musty hay. It was used during World War I against troops.

4. **What is the central atom in \(\text{SCl}_2\text{O}\)?**

Hint: Sulfur is the central atom.

**Skill:**
Identifying the central atom is a good start to drawing a structure:

5. **What is the number of valence electrons in sulfur?**

Hint: Sulfur has 6 valence electrons.

**Skill:**
Give the number of valence electrons of any main-group element.

6. **What is the number of lone pair electrons around the central atom \(\text{S}\) in \(\text{SCl}_2\text{O}\)?**

Hint: There is one lone electron pair.

**Skill:**
Draw a Lewis dot structure, and express in the form \(\text{SCl}_2\text{O}\) or \(\text{SCl}_2\text{OE}\).

7. **What is the number of lone pairs of electrons around \(\text{O}\) in \(\text{H}_2\text{O}\)?**

Hint: There are two lone electron pairs.
Skill:
The structure is

\[
\begin{array}{c}
H \\
> O \\
H
\end{array}
\]

8. **How many lone electron pairs are there around \(\text{C}\) in \(\text{CO}_2\)?**

Hint: There is no lone electron pair for carbon dioxide.

Skill:
From the structure of \(\text{O=C=O}\), figure out the number of lone electron pairs. \(\text{CO}_2\) is linear; so is \(\text{H-CN}\).

9. **What is the molecular shape of \(\text{ClF}_3\) (chlorine-trifluoride)?**

Hint: The molecule has a T shape.

Skill:
Predict the shape of a molecule \(\text{ClF}_3\) or \(\text{ClF}_3E_2\).

\[
\begin{array}{c}
F \\
| \\
F---\text{Cl}---F
\end{array}
\]

10. **What is the bond angle (in degrees) in a \(\text{CH}_4\) molecule?**

Hint: The angle for ideal tetrahedral molecule is 109.5 degrees.

Skill:
Calculate bond angles from the geometry.

11. **What is the shape of \(\text{SF}_6\)? Give a geometric term for the configuration of the 6 \(\text{F}\)'s around \(\text{S}\).**

Hint: The geometrical shape is octahedral.

Skill:
Apply terms linear, T shape, seesaw, trigonal planar, trigonal bipyramidal, tetrahedral, octahedral etc. to describe the geometric shapes of molecules.

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**Contributors and Attributions**

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